#### Hybrid Continuous Mixtures of Probabilistic Circuits

Dewi Batista July 18, 2025

#### Outline

- Part 1: Probabilistic models
- Part 2: Probabilistic circuits (PCs)
- Part 3: Continuous mixtures of PCs (CMPCs)
- Part 4: Hybrid CMPCs

#### Notation

Probability density/mass functions are denoted by p; if parameterised then  $p_{\Theta}$ .

#### **Notation**

Probability density/mass functions are denoted by p; if parameterised then  $p_{\Theta}$ .

#### Terminology

Probability density/mass functions are referred to as probability functions.

#### **Notation**

Probability density/mass functions are denoted by p; if parameterised then  $p_{\Theta}$ .

#### Terminology

Probability density/mass functions are referred to as probability functions.

#### More notation

The sample space of a set of random variables  $\mathbf{X} = \{X_1, \dots, X_n\}$  is denoted  $\Omega_{\mathbf{X}}$ .

We often write x to denote a realisation  $(x_1, \ldots, x_n) \in \Omega_X$ .

#### **Definition**

A generative probabilistic model  $(\mathbf{X},p_{\Theta})$  consists of a finite set  $\mathbf{X}=\{X_1,\ldots,X_n\}$  of random variables and a representation

$$p_{\Theta}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$$

of a probability function over X parameterised by a parameter tuple  $\Theta$ .

Dewi Batista Hybrid CMPCs July 18, 2025 3 / 22

#### **Definition**

A generative probabilistic model  $(\mathbf{X},p_{\Theta})$  consists of a finite set  $\mathbf{X}=\{X_1,\ldots,X_n\}$  of random variables and a representation

$$p_{\Theta}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$$

of a probability function over X parameterised by a parameter tuple  $\Theta$ .

#### Probabilistic queries:

- Evidence (evi):  $p_{\Theta}(\mathbf{x})$  where  $\mathbf{x} \in \Omega_{\mathbf{X}}$
- ullet Marginal (marg):  $p_{\Theta}(\mathbf{x}')$  where  $\mathbf{x}' \in \Omega_{\mathbf{X}'}$  with  $\mathbf{X}' \subset \mathbf{X}$
- ullet Sampling (samp): a stochastic procedure that yields some  ${f x}\in\Omega_{f X}$

Dewi Batista Hybrid CMPCs July 18, 2025 3 / 22

#### Definition

A generative probabilistic model  $(\mathbf{X}, p_{\Theta})$  consists of a finite set  $\mathbf{X} = \{X_1, \dots, X_n\}$  of random variables and a representation

$$p_{\Theta}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$$

of a probability function over X parameterised by a parameter tuple  $\Theta$ .

#### Probabilistic queries:

- Evidence (evi):  $p_{\Theta}(\mathbf{x})$  where  $\mathbf{x} \in \Omega_{\mathbf{X}}$
- Marginal (marg):  $p_{\Theta}(\mathbf{x}')$  where  $\mathbf{x}' \in \Omega_{\mathbf{X}'}$  with  $\mathbf{X}' \subset \mathbf{X}$
- Sampling (samp): a stochastic procedure that yields some  $\mathbf{x} \in \Omega_{\mathbf{X}}$

Dewi Batista Hybrid CMPCs July 18, 2025 3/22

#### Definition

A generative probabilistic model  $(\mathbf{X}, p_{\Theta})$  consists of a finite set  $\mathbf{X} = \{X_1, \dots, X_n\}$  of random variables and a representation

$$p_{\Theta}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$$

of a probability function over X parameterised by a parameter tuple  $\Theta$ .

#### Probabilistic queries:

- Evidence (evi):  $p_{\Theta}(\mathbf{x})$  where  $\mathbf{x} \in \Omega_{\mathbf{X}}$
- Marginal (marg):  $p_{\Theta}(\mathbf{x}')$  where  $\mathbf{x}' \in \Omega_{\mathbf{X}'}$  with  $\mathbf{X}' \subset \mathbf{X}$
- Sampling (samp): a stochastic procedure that yields some  $\mathbf{x} \in \Omega_{\mathbf{X}}$

Hybrid CMPCs July 18, 2025 3 / 22

#### Definition

A generative probabilistic model  $(\mathbf{X},p_{\Theta})$  consists of a finite set  $\mathbf{X}=\{X_1,\ldots,X_n\}$  of random variables and a representation

$$p_{\Theta}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$$

of a probability function over X parameterised by a parameter tuple  $\Theta$ .

#### Probabilistic queries:

- Evidence (evi):  $p_{\Theta}(\mathbf{x})$  where  $\mathbf{x} \in \Omega_{\mathbf{X}}$ 
  - Marginal (marg):  $p_{\Theta}(\mathbf{x}')$  where  $\mathbf{x}' \in \Omega_{\mathbf{X}'}$  with  $\mathbf{X}' \subset \mathbf{X}$
  - ullet Sampling (samp): a stochastic procedure that yields some  ${f x}\in\Omega_{f X}$

Dewi Batista Hybrid CMPCs July 18, 2025 3 / 22

#### Definition

A generative probabilistic model  $(\mathbf{X},p_{\Theta})$  consists of a finite set  $\mathbf{X}=\{X_1,\ldots,X_n\}$  of random variables and a representation

$$p_{\Theta}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$$

of a probability function over X parameterised by a parameter tuple  $\Theta$ .

#### Probabilistic queries:

- Evidence (evi):  $p_{\Theta}(\mathbf{x})$  where  $\mathbf{x} \in \Omega_{\mathbf{X}}$
- Marginal (marg):  $p_{\Theta}(\mathbf{x}')$  where  $\mathbf{x}' \in \Omega_{\mathbf{X}'}$  with  $\mathbf{X}' \subset \mathbf{X}$
- ullet Sampling (samp): a stochastic procedure that yields some  ${f x}\in\Omega_{f X}$

#### Terminology

Probabilistic queries are answered.

#### Gaussian mixtures

A univariate Gaussian mixture  $(\mathbf{X}, p_{(K,\mu,\sigma,\mathbf{w})})$  is a probabilistic model in which  $\mathbf{X}=\{X\}$ , so  $\Omega_{\mathbf{X}}=\mathbb{R}$ ,  $\mathbf{x}=x$  and

$$p_{\Theta}(\mathbf{x}) = \sum_{k=1}^{K} w_k \mathcal{N}(\mathbf{x}|\mu_k, \sigma_k^2)$$

where  $\Theta=(K,\mu,\sigma,\mathbf{w})$  consists of the number of components  $K\in\mathbb{N}$ , means  $\mu=(\mu_1,\dots,\mu_K)\in\mathbb{R}^K$ , standard deviations  $\sigma=(\sigma_1,\dots,\sigma_K)\in\mathbb{R}^K_{\geq 0}$  and weights  $\mathbf{w}=(w_1,\dots,w_K)\in\mathbb{R}^K_{\geq 0}$  with  $\sum_{k=1}^K w_k=1$ .

Dewi Batista Hybrid CMPCs July 18, 2025 4 / 22

#### Gaussian mixtures

A univariate Gaussian mixture  $(\mathbf{X}, p_{(K,\mu,\sigma,\mathbf{w})})$  is a probabilistic model in which  $\mathbf{X}=\{X\}$ , so  $\Omega_{\mathbf{X}}=\mathbb{R}$ ,  $\mathbf{x}=x$  and

$$p_{\Theta}(\mathbf{x}) = \sum_{k=1}^{K} w_k \mathcal{N}(\mathbf{x}|\mu_k, \sigma_k^2)$$

#### Gaussian mixtures

A univariate Gaussian mixture  $(\mathbf{X}, p_{(K,\mu,\sigma,\mathbf{w})})$  is a probabilistic model in which  $\mathbf{X}=\{X\}$ , so  $\Omega_{\mathbf{X}}=\mathbb{R}$ ,  $\mathbf{x}=x$  and

$$p_{\Theta}(\mathbf{x}) = \sum_{k=1}^{K} w_k \mathcal{N}(\mathbf{x}|\mu_k, \sigma_k^2)$$

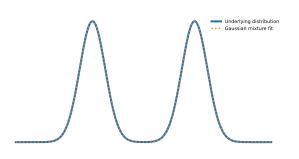


Figure: A Gaussian mixture with K=2 fit to a bimodal distribution.

#### Gaussian mixtures

A univariate Gaussian mixture  $(\mathbf{X}, p_{(K,\mu,\sigma,\mathbf{w})})$  is a probabilistic model in which  $\mathbf{X}=\{X\}$ , so  $\Omega_{\mathbf{X}}=\mathbb{R}$ ,  $\mathbf{x}=x$  and

$$p_{\Theta}(\mathbf{x}) = \sum_{k=1}^{K} w_k \mathcal{N}(\mathbf{x}|\mu_k, \sigma_k^2)$$

#### The class of univariate Gaussian mixtures

We often talk about classes of probabilistic models. For example,

$$\mathsf{GM}(\mathbf{X}) = \left\{ p_{(K,\mu,\sigma,\mathbf{w})} : K \in \mathbb{N}, \mu \in \mathbb{R}^K, \sigma, \mathbf{w} \in \mathbb{R}^K_{>0} \text{ and } \sum_{k=1}^K w_k = 1 \right\}$$

 Dewil Batista
 Hybrid CMPCs
 July 18, 2025
 4 / 22

- Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- **Solution** Exp.-efficiency: how efficiently a model class can fit distributions

- Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- **Solution** Exp.-efficiency: how efficiently a model class can fit distributions

- **1** Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- **©** Exp.-efficiency: how efficiently a model class can fit distributions

- Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- **Solution** Exp.-efficiency: how efficiently a model class can fit distributions

The trifecta of goodness for a class of probabilistic models:

- **Tractability**: how efficiently the model class can answer queries
- 2 Expressivity: how precisely a model class can fit distributions
- **Solution** Exp.-efficiency: how efficiently a model class can fit distributions

Model\Probabilistic query	samp	evi	marg
Bayesian networks [5]	<b>√</b>	<b>√</b>	Х
Gaussian mixtures	✓	<b>√</b>	<b>√</b>
Probabilistic circuits	<b>√</b>	<b>√</b>	<b>√</b>

Table: The tractability of classes of probabilistic models.

- Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- **Solution** Exp.-efficiency: how efficiently a model class can fit distributions

- 1 Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- Exp.-efficiency: how efficiently a model class can fit distributions

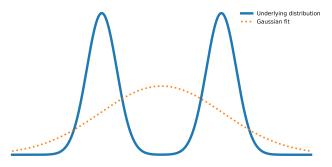


Figure: A Gaussian fit to a bimodal distribution.

- **1** Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- Exp.-efficiency: how efficiently a model class can fit distributions

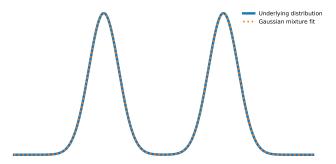


Figure: A Gaussian mixture fit to a bimodal distribution.

- 1 Tractability: how efficiently the model class can answer queries
- ② Expressivity: how precisely a model class can fit distributions
- Exp.-efficiency: how efficiently a model class can fit distributions



Figure: A complex distribution.

- 1 Tractability: how efficiently the model class can answer queries
- 2 Expressivity: how precisely a model class can fit distributions
- Exp.-efficiency: how efficiently a model class can fit distributions

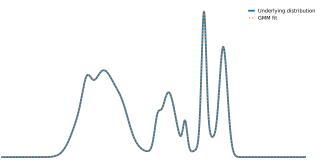


Figure: A 20-component Gaussian mixture fit to a complex distribution.

The trifecta of goodness for a class of probabilistic models:

- 1 Tractability: how efficiently the model class can answer queries
- ② Expressivity: how precisely a model class can fit distributions
- **3** Exp.-efficiency: how efficiently a model class can fit distributions

#### Universal distribution approximation

"A Gaussian mixture model is a universal approximator of densities, in the sense that any smooth density can be approximated with any specific non-zero amount of error by a Gaussian mixture model with enough components." [3, Page 67]

The class of Gaussian mixtures has perfect expressivity!

The trifecta of goodness for a class of probabilistic models:

- 1 Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- **SEXP.-efficiency**: how efficiently a model class can fit distributions

#### Universal distribution approximation

"A Gaussian mixture model is a universal approximator of densities, in the sense that any smooth density can be approximated with any specific non-zero amount of error by a Gaussian mixture model with enough components." [3, Page 67]

The class of Gaussian mixtures has perfect expressivity!

- 1 Tractability: how efficiently the model class can answer queries
- 2 Expressivity: how precisely a model class can fit distributions
- **©** Exp.-efficiency: how efficiently a model class can fit distributions

The trifecta of goodness for a class of probabilistic models:

- 1 Tractability: how efficiently the model class can answer queries
- 2 Expressivity: how precisely a model class can fit distributions
- **SEXP.-efficiency**: how efficiently a model class can fit distributions

**Example:** The number of components in a Gaussian mixture needed to fit complex distributions is high in practice, i.e. low expressive-efficiency!

The trifecta of goodness for a class of probabilistic models:

- **1** Tractability: how efficiently the model class can answer queries
- 2 Expressivity: how precisely a model class can fit distributions
- **Solution Exp.-efficiency**: how efficiently a model class can fit distributions

**Example:** The number of components in a Gaussian mixture needed to fit complex distributions is high in practice, i.e. low expressive-efficiency!

Is there a class of probabilistic models which offers a bit of all three?

The trifecta of goodness for a class of probabilistic models:

- **1** Tractability: how efficiently the model class can answer queries
- Expressivity: how precisely a model class can fit distributions
- **3** Exp.-efficiency: how efficiently a model class can fit distributions

**Example:** The number of components in a Gaussian mixture needed to fit complex distributions is high in practice, i.e. low expressive-efficiency!

Is there a class of probabilistic models which offers a bit of all three?

Probabilistic circuits (PCs)!

#### Beginning of overview

A probabilistic circuit  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a generative probabilistic model whose parameter tuple  $\Theta = (\mathcal{G}, \mathbf{w}, \theta)$  consists of a weighted graph  $\mathcal{G}$ , tuple of weights  $\mathbf{w}$  and a parameter tuple  $\theta$  pertaining to the probability functions of its input nodes.

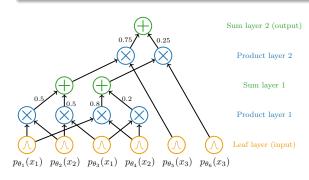


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

#### Beginning of overview

A probabilistic circuit  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a generative probabilistic model whose parameter tuple  $\Theta = (\mathcal{G}, \mathbf{w}, \theta)$  consists of a weighted graph  $\mathcal{G}$ , tuple of weights  $\mathbf{w}$  and a parameter tuple  $\theta$  pertaining to the probability functions of its input nodes.

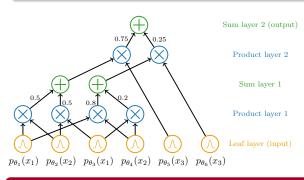


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

#### Comment on weights

The weights of the edges pointing to a given sum node must sum to 1.

Dewi Batista Hybrid CMPCs July 18, 2025 6 / 22

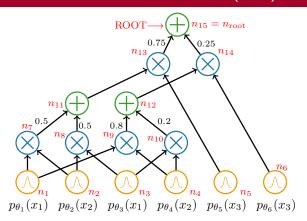
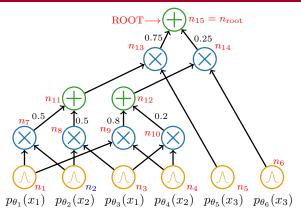


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.



Associated function of node  $n_2$ :

$$p_{n_2}(x_2) = p_{\theta_2}(x_2)$$

Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

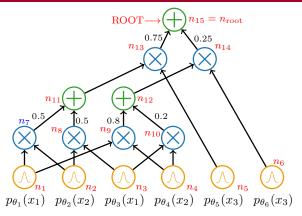


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

Associated function of node  $n_7$ :

$$p_{n_7}(x_1, x_2) = p_{\theta_1}(x_1)p_{\theta_2}(x_2)$$

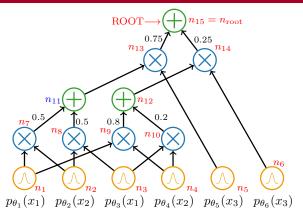


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

Associated function of node  $n_{11}$ :

$$p_{n_{11}}(x_1, x_2) = 0.5p_{n_7}(x_1, x_2) + 0.5p_{n_8}(x_1, x_2)$$
  
=  $0.5p_{\theta_1}(x_1)p_{\theta_2}(x_2) + 0.5p_{\theta_3}(x_1)p_{\theta_2}(x_2)$ 

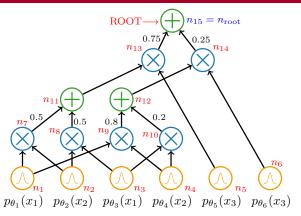
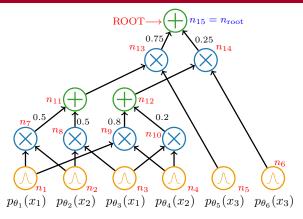


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

Associated function of node  $n_{15}$  (the root node):

$$\begin{split} p_{n_{15}}(x_1,x_2,x_3) &= \frac{15}{40} p_{\theta_1}(x_1) p_{\theta_2}(x_2) p_{\theta_5}(x_3) + \frac{15}{40} p_{\theta_3}(x_1) p_{\theta_2}(x_2) p_{\theta_5}(x_3) \\ &+ \frac{8}{40} p_{\theta_1}(x_1) p_{\theta_4}(x_2) p_{\theta_6}(x_3) + \frac{2}{40} p_{\theta_3}(x_1) p_{\theta_4}(x_2) p_{\theta_6}(x_3) \end{split}$$



What is  $p_{(\mathcal{G}, \mathbf{w}, \theta)}$  for a PC?

Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

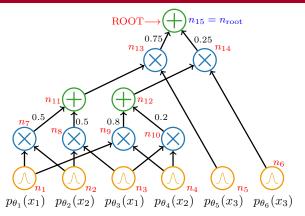


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

What is  $p_{(\mathcal{G},\mathbf{w},\theta)}$  for a PC? The associated function of the root node,  $n_{\mathsf{root}}!$ 

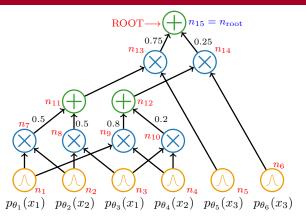
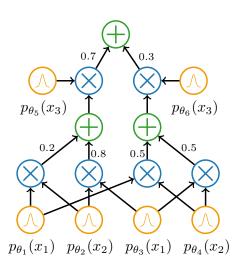


Figure: A PC over  $\mathbf{X} = \{X_1, X_2, X_3\}$  with six input nodes.

Input nodes in orange, product nodes in blue and sum nodes in green.

What is  $p_{(\mathcal{G},\mathbf{w},\theta)}$  for a PC? The associated function of the root node,  $n_{\mathsf{root}}!$ 

$$\begin{split} p_{n_{15}}(x_1,x_2,x_3) &= \frac{15}{40} p_{\theta_1}(x_1) p_{\theta_2}(x_2) p_{\theta_5}(x_3) + \frac{15}{40} p_{\theta_3}(x_1) p_{\theta_2}(x_2) p_{\theta_5}(x_3) \\ &+ \frac{8}{40} p_{\theta_1}(x_1) p_{\theta_4}(x_2) p_{\theta_6}(x_3) + \frac{2}{40} p_{\theta_3}(x_1) p_{\theta_4}(x_2) p_{\theta_6}(x_3) \end{split}$$



## Computational graph G:

Displayed to the left

## Weights w:

Displayed to the left

### Input nodes:

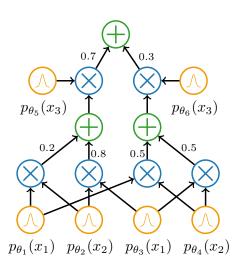
$$p_{\theta_i}(x) = \text{Ber}(x|\theta_i) \text{ with}$$

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$ 

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

$$p_{(\mathcal{G}, \mathbf{w}, \theta)}(0, 1, 1) = 7$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

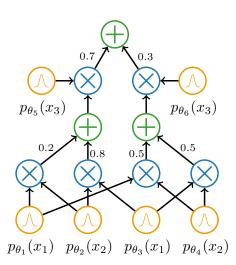
$$p_{\theta_i}(x) = \text{Ber}(x|\theta_i) \text{ with}$$

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$ 

### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

$$p_{(\mathcal{G}, \mathbf{w}, \theta)}(0, 1, 1) = 7$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

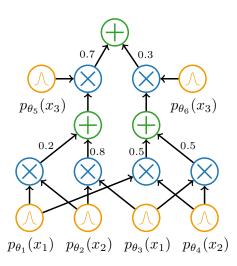
$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

$$p_{(\mathcal{G},\mathbf{w},\theta)}(0,1,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3 \quad \theta_2 = 0.2 \quad \theta_3 = 0.1$$

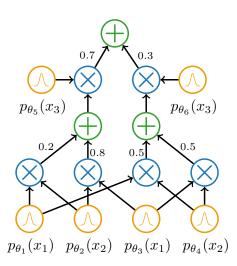
$$\theta_4 = 0.6 \quad \theta_5 = 0.5 \quad \theta_6 = 0.4$$

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

### **Evidence query:**

$$p_{(\mathcal{G}, \mathbf{w}, \theta)}(0, 1, 1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

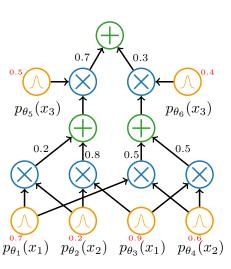
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

### **Evidence query:**

$$p_{(G,\mathbf{w},\theta)}(0,1,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

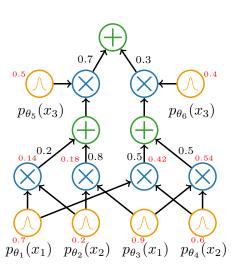
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

### **Evidence query:**

$$p_{(G,\mathbf{w},\theta)}(0,1,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

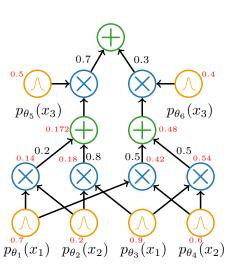
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

### **Evidence query:**

$$p_{(G,\mathbf{w},\theta)}(0,1,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

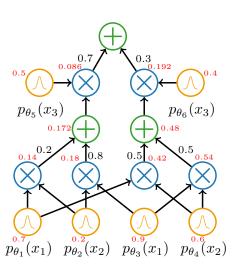
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

### **Evidence query:**

$$p_{(G,\mathbf{w},\theta)}(0,1,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

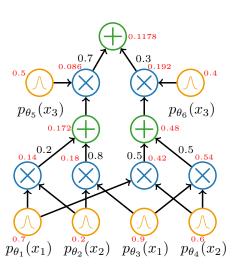
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

### **Evidence query:**

$$p_{(\mathcal{G}, \mathbf{w}, \theta)}(0, 1, 1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

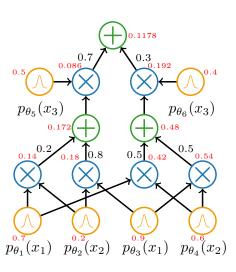
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

### **Evidence query:**

$$p_{(G,\mathbf{w},\theta)}(0,1,1) = ?$$



### Computational graph G:

Displayed to the left

## Weights w:

Displayed to the left

### Input nodes:

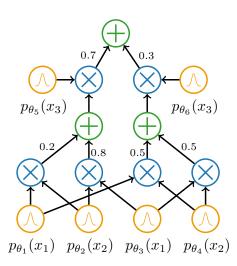
$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_2, x_3) = (0, 1, 1)$$

$$p_{(G,\mathbf{w},\theta)}(0,1,1) = 0.1178$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

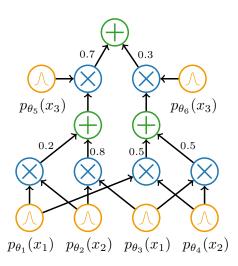
### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

$$(x_1, x_3) = (0, 1)$$

$$p_{(G,\mathbf{w},\theta)}(0,1) = 1$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

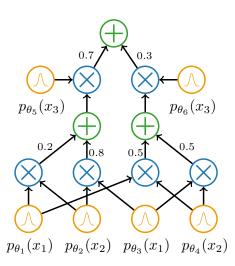
### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

$$(x_1, x_3) = (0, 1)$$

$$p_{(\mathcal{G},\mathbf{w},\theta)}(0,1) = 1$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

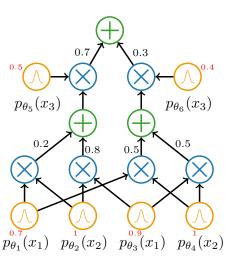
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_3) = (0, 1)$$

### Marginal query:

$$p_{(G,\mathbf{w},\theta)}(0,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

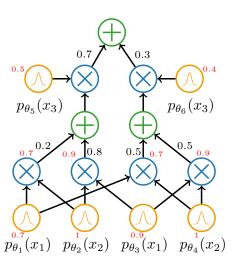
$$p_{\theta_i}(x) = \operatorname{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_3) = (0, 1)$$

$$p_{(G,\mathbf{w},\theta)}(0,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \operatorname{Ber}(x|\theta_i)$$
 with

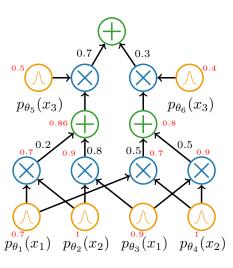
$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_3) = (0, 1)$$

### Marginal query:

$$p_{(G,\mathbf{w},\theta)}(0,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

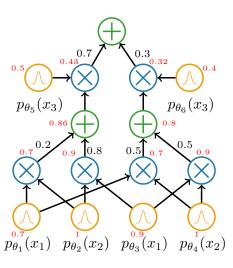
$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_3) = (0, 1)$$

$$p_{(G,\mathbf{w},\theta)}(0,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

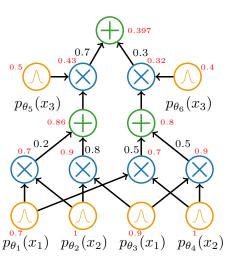
$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_3) = (0, 1)$$

$$p_{(G,\mathbf{w},\theta)}(0,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

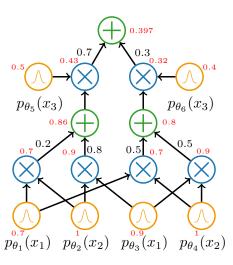
$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_3) = (0, 1)$$

$$p_{(G,\mathbf{w},\theta)}(0,1) = ?$$



### Computational graph G:

Displayed to the left

### Weights w:

Displayed to the left

### Input nodes:

$$p_{\theta_i}(x) = \mathrm{Ber}(x|\theta_i)$$
 with

$$\theta_1 = 0.3$$
  $\theta_2 = 0.2$   $\theta_3 = 0.1$   
 $\theta_4 = 0.6$   $\theta_5 = 0.5$   $\theta_6 = 0.4$ 

#### Realisation:

$$(x_1, x_3) = (0, 1)$$

$$p_{(G,\mathbf{w},\theta)}(0,1) = 0.397$$

- Tractability: how efficiently the model class can answer queries
  evi and marg queries are linear in the number of edges in the PC!
  - 2 Expressivity: how precisely a model class can fit distributions

At least as expressive as Gaussian mixtures which have perfect expressivity!

Expressive-efficiency: how efficiently a model class can fit distributions

Entirely empirically-motivated

- Tractability: how efficiently the model class can answer queriesevi and marg queries are linear in the number of edges in the PC!
  - Expressivity: how precisely a model class can fit distributions

At least as expressive as Gaussian mixtures which have perfect expressivity!

Expressive-efficiency: how efficiently a model class can fit distributions

Entirely empirically-motivated

- Tractability: how efficiently the model class can answer queriesevi and marg queries are linear in the number of edges in the PC!
  - Expressivity: how precisely a model class can fit distributions

At least as expressive as Gaussian mixtures which have perfect expressivity!

Expressive-efficiency: how efficiently a model class can fit distributions

Entirely empirically-motivated

- Tractability: how efficiently the model class can answer queriesevi and marg queries are linear in the number of edges in the PC!
  - Expressivity: how precisely a model class can fit distributions

At least as expressive as Gaussian mixtures which have perfect expressivity!

Expressive-efficiency: how efficiently a model class can fit distributions

Entirely empirically-motivated

## Learning PCs (so $\mathcal{G}$ , w and $\theta$ ) from data

Tons of methods. Some inspired by learning Bayesian networks from data.

# Part 2: Probabilistic circuits (applications)

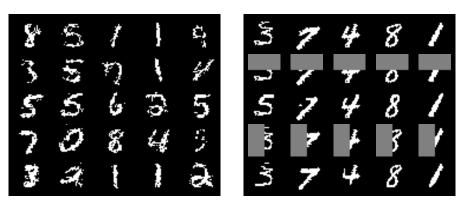


Figure: Sampling (left) and in-painting (right). Taken from [2, Figure 2].

 Dewi Batista
 Hybrid CMPCs
 July 18, 2025
 10 / 22

# Part 2: Probabilistic circuits (applications)

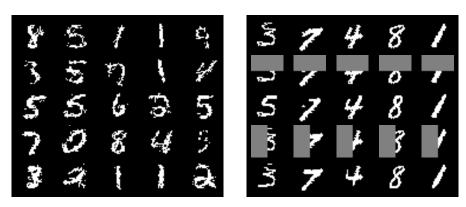


Figure: Sampling (left) and in-painting (right). Taken from [2, Figure 2].

### Classification

Assign label according to  $\arg\max_{y\in\Omega_Y}p(y|\mathbf{x})=\arg\max_{y\in\Omega_Y}p(\mathbf{x},y).$ 

#### Definition

A continuous mixture of probabilistic circuits (CMPC) is a PC of the form

$$p(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}|\mathbf{z}_i)$$

where  $N \in \mathbb{N}$ ,  $\mathbf{z}_1, \dots, \mathbf{z}_N \sim p(\mathbf{z})$  with  $\mathbf{Z} \sim \mathcal{N}(0, I_d)$  for some latent dimension  $d \in \{2, \dots, 16\}$ . A PC is fit to each component distribution  $p_{\phi}(\mathbf{x}|\mathbf{z})$  and parameterised according to  $\phi(\mathbf{z})$  where  $\phi$  is a decoder with  $\text{dom}(\phi) = \Omega_{\mathbf{Z}}$ .

#### Definition

A continuous mixture of probabilistic circuits (CMPC) is a PC of the form

$$p(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}|\mathbf{z}_i)$$

where  $N \in \mathbb{N}$ ,  $\mathbf{z}_1, \dots, \mathbf{z}_N \sim p(\mathbf{z})$  with  $\mathbf{Z} \sim \mathcal{N}(0, I_d)$  for some latent dimension  $d \in \{2, \dots, 16\}$ . A PC is fit to each component distribution  $p_{\phi}(\mathbf{x}|\mathbf{z})$  and parameterised according to  $\phi(\mathbf{z})$  where  $\phi$  is a decoder with  $\text{dom}(\phi) = \Omega_{\mathbf{Z}}$ .

Answer: Choose a very simple sub-class of PC structures for each component distribution  $p_{\phi}(\mathbf{x}|\mathbf{z})$ , e.g. a fully-factorised model

$$p_{\phi}(\mathbf{x}|\mathbf{z}) = \prod_{i=1}^{n} p_{\phi}(x_i|\mathbf{z}).$$

#### Definition

A continuous mixture of probabilistic circuits (CMPC) is a PC of the form

$$p(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x} | \mathbf{z}_i)$$

where  $N \in \mathbb{N}$ ,  $\mathbf{z}_1, \dots, \mathbf{z}_N \sim p(\mathbf{z})$  with  $\mathbf{Z} \sim \mathcal{N}(0, I_d)$  for some latent dimension  $d \in \{2, \dots, 16\}$ . A PC is fit to each component distribution  $p_{\phi}(\mathbf{x}|\mathbf{z})$  and parameterised according to  $\phi(\mathbf{z})$  where  $\phi$  is a decoder with dom $(\phi) = \Omega_{\mathbf{Z}}$ .

### Terminology

CMPCs are a sub-class of discrete mixtures of PCs. Not 'continuous mixtures'...

More on the simple PC structures fit to the N component distributions:

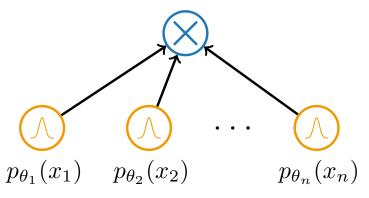


Figure: A fully-factorised model (FFM),  $p(\mathbf{x}) = \prod_{i=1}^n p_{\theta_i}(x_i)$ , as a PC.

More on the simple PC structures fit to the N component distributions:

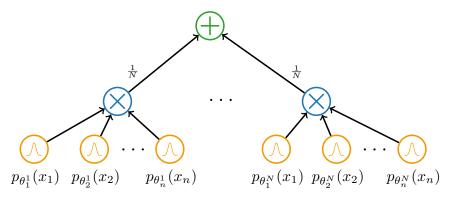


Figure: A CMPC with FFMs fit to the N component distributions.

 Dewi Batista
 Hybrid CMPCs
 July 18, 2025
 12 / 22

More on the simple PC structures fit to the N component distributions:

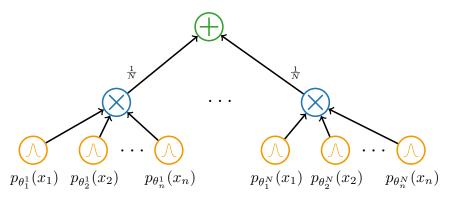


Figure: A CMPC with FFMs fit to the N component distributions.

#### No elaborate PC structure overall?

More elaborate sub-classes of PCs could be used. Required compute increases.

#### Example (Binary MNIST):

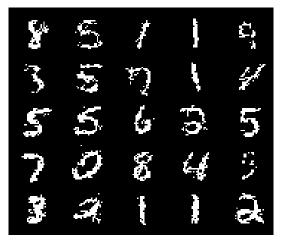


Figure: Samples of Binary MNIST. 28 by 28 (784 pixels) each.

Example (Binary MNIST): Fit an FFM to each component distribution. For component  $i \in \{1, \dots, N\}$ , conditioned on sampled latent  $\mathbf{z}_i \sim p(\mathbf{z})$ , pixel distributions are independent Bernoulli distributions, i.e.

$$p_{\phi}(x_1, \dots, x_{784} | \mathbf{z}_i) = \prod_{j=1}^{784} \mathsf{Ber}(x_j | \phi(\mathbf{z}_i))$$

and so a CMPC with N=100 components is given by

$$p_{\phi}(x_1, \dots, x_{784}) = \frac{1}{100} \sum_{i=1}^{100} p_{\phi}(x_1, \dots, x_{784} | \mathbf{z}_i)$$
$$= \frac{1}{100} \sum_{i=1}^{100} \left[ \prod_{j=1}^{784} \operatorname{Ber}(x_j | \phi(\mathbf{z}_i)) \right].$$

If latent dimension d=16 then  $\mathbf{Z} \sim \mathcal{N}(0, I_{16})$  and  $\phi: \mathbb{R}^{16} \to [0, 1]^{784}$ .

Example (Binary MNIST): Fit an FFM to each component distribution. For component  $i \in \{1, \dots, N\}$ , conditioned on sampled latent  $\mathbf{z}_i \sim p(\mathbf{z})$ , pixel distributions are independent Bernoulli distributions, i.e.

$$p_{\phi}(x_1, \dots, x_{784} | \mathbf{z}_i) = \prod_{j=1}^{784} \mathsf{Ber}(x_j | \phi(\mathbf{z}_i))$$

and so a CMPC with N=100 components is given by

$$p_{\phi}(x_1, \dots, x_{784}) = \frac{1}{100} \sum_{i=1}^{100} p_{\phi}(x_1, \dots, x_{784} | \mathbf{z}_i)$$
$$= \frac{1}{100} \sum_{i=1}^{100} \left[ \prod_{j=1}^{784} \operatorname{Ber}(x_j | \phi(\mathbf{z}_i)) \right].$$

If latent dimension d=16 then  $\mathbf{Z} \sim \mathcal{N}(0, I_{16})$  and  $\phi: \mathbb{R}^{16} \to [0, 1]^{784}$ .

Example (Binary MNIST): Fit an FFM to each component distribution. For component  $i \in \{1, \dots, N\}$ , conditioned on sampled latent  $\mathbf{z}_i \sim p(\mathbf{z})$ , pixel distributions are independent Bernoulli distributions, i.e.

$$p_{\phi}(x_1, \dots, x_{784} | \mathbf{z}_i) = \prod_{j=1}^{784} \mathsf{Ber}(x_j | \phi(\mathbf{z}_i))$$

and so a CMPC with N=100 components is given by

$$p_{\phi}(x_1, \dots, x_{784}) = \frac{1}{100} \sum_{i=1}^{100} p_{\phi}(x_1, \dots, x_{784} | \mathbf{z}_i)$$
$$= \frac{1}{100} \sum_{i=1}^{100} \left[ \prod_{j=1}^{784} \operatorname{Ber}(x_j | \phi(\mathbf{z}_i)) \right].$$

If latent dimension d=16 then  $\mathbf{Z} \sim \mathcal{N}(0, I_{16})$  and  $\phi: \mathbb{R}^{16} \to [0, 1]^{784}$ .

#### How might we fit the decoder $\phi$ ?

Task-dependent! For Binary MNIST, a multi-layer perceptron (MLP) works well. So an MLP encoding  $\phi: \mathbb{R}^d \to [0,1]^{784}$  where d is the latent dimension.

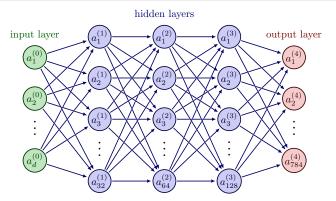


Figure: An MLP with d input nodes and 784 output nodes.

How to learn  $\phi$ ? Maximum likelihood! Let  $\{\mathbf{x}_j\}_{j=1}^M$  denote training data. Choose  $N_{\text{train}}$  and latent dimension  $d \in \{2, \dots, 16\}$  chosen a priori.

Sample  $\mathbf{z}_1, \dots \mathbf{z}_{N_{\mathsf{train}}} \sim p(\mathbf{z})$ , where  $\mathbf{Z} \sim \mathcal{N}(0, I_d)$ , and compute

$$\begin{split} \arg\min_{\phi} \mathcal{L}(\phi) &= \arg\min_{\phi} \mathsf{NLL}(\phi) \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log(p(\mathbf{x})) \right] \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log\left(\frac{1}{N_{\mathsf{train}}} \sum_{i=1}^{N_{\mathsf{train}}} p_{\phi}(\mathbf{x}_{j} | \mathbf{z}_{i}) \right) \right] \end{split}$$

via gradient descent.

**Note:** If learned in batches, new  $\mathbf{z}_1, \dots, \mathbf{z}_{N_{\text{train}}} \sim p(\mathbf{z})$  for each batch.

Dewi Batista Hybrid CMPCs July 18, 2025

How to learn  $\phi$ ? Maximum likelihood! Let  $\{\mathbf{x}_j\}_{j=1}^M$  denote training data. Choose  $N_{\text{train}}$  and latent dimension  $d \in \{2, \dots, 16\}$  chosen a priori.

Sample  $\mathbf{z}_1, \dots \mathbf{z}_{N_{\mathsf{train}}} \sim p(\mathbf{z})$ , where  $\mathbf{Z} \sim \mathcal{N}(0, I_d)$ , and compute

$$\begin{split} \arg\min_{\phi} \mathcal{L}(\phi) &= \arg\min_{\phi} \mathsf{NLL}(\phi) \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log(p(\mathbf{x})) \right] \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log\left(\frac{1}{N_{\mathsf{train}}} \sum_{i=1}^{N_{\mathsf{train}}} p_{\phi}(\mathbf{x}_{j} | \mathbf{z}_{i}) \right) \right] \end{split}$$

via gradient descent.

**Note:** If learned in batches, new  $\mathbf{z}_1, \dots, \mathbf{z}_{N_{\text{train}}} \sim p(\mathbf{z})$  for each batch.

Dewi Batista Hybrid CMPCs July 18, 2025

How to learn  $\phi$ ? Maximum likelihood! Let  $\{\mathbf{x}_j\}_{j=1}^M$  denote training data. Choose  $N_{\text{train}}$  and latent dimension  $d \in \{2, \dots, 16\}$  chosen a priori.

Sample  $\mathbf{z}_1, \dots \mathbf{z}_{N_{\mathsf{train}}} \sim p(\mathbf{z})$ , where  $\mathbf{Z} \sim \mathcal{N}(0, I_d)$ , and compute

$$\begin{split} \arg\min_{\phi} \mathcal{L}(\phi) &= \arg\min_{\phi} \mathsf{NLL}(\phi) \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log(p(\mathbf{x})) \right] \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log\left(\frac{1}{N_{\mathsf{train}}} \sum_{i=1}^{N_{\mathsf{train}}} p_{\phi}(\mathbf{x}_{j} | \mathbf{z}_{i}) \right) \right] \end{split}$$

via gradient descent.

**Note:** If learned in batches, new  $\mathbf{z}_1,\dots,\mathbf{z}_{N_{\text{train}}} \sim p(\mathbf{z})$  for each batch.

Dewi Batista Hybrid CMPCs July 18, 2025

After learning  $\phi$ : Choose  $N_{\mathsf{test}} \in \mathbb{N}$ , sample  $\mathbf{z}_1, \dots, \mathbf{z}_{N_{\mathsf{test}}} \sim p(\mathbf{z})$ , compute  $\phi(\mathbf{z}_1), \dots, \phi(\mathbf{z}_{N_{\mathsf{test}}})$  and compile

$$p(\mathbf{x}) = \frac{1}{N_{\text{test}}} \sum_{i=1}^{N_{\text{test}}} p_{\phi}(\mathbf{x} | \mathbf{z}_i).$$

Note: Component distributions are parameterised by a shared decoder, so an N-component discrete mixture model is at least as expressive as an N-component CMPC. So what is useful about CMPCs?

After learning  $\phi$ : Choose  $N_{\mathsf{test}} \in \mathbb{N}$ , sample  $\mathbf{z}_1, \dots, \mathbf{z}_{N_{\mathsf{test}}} \sim p(\mathbf{z})$ , compute  $\phi(\mathbf{z}_1), \dots, \phi(\mathbf{z}_{N_{\mathsf{test}}})$  and compile

$$p(\mathbf{x}) = \frac{1}{N_{\text{test}}} \sum_{i=1}^{N_{\text{test}}} p_{\phi}(\mathbf{x} | \mathbf{z}_i).$$

Note: Component distributions are parameterised by a shared decoder, so an N-component discrete mixture model is at least as expressive as an N-component CMPC. So what is useful about CMPCs?

Note: Component distributions are parameterised by a shared decoder, so an N-component discrete mixture model is at least as expressive as an N-component CMPC. So what is useful about CMPCs?

Note: Component distributions are parameterised by a shared decoder, so an N-component discrete mixture model is at least as expressive as an N-component CMPC. So what is useful about CMPCs?

Dataset	BestPC	$cm(S_F)$	$cm(S_CLT)$	$LO(cm(S_CLT))$	Dataset	BestPC	$cm(S_F)$	$cm(S_CLT)$	$LO(cm(S_CLT))$
accid.	26.74	33.27	28.69	28.81	jester	52.46	51.93	51.94	51.94
ad	16.07	18.71	14.76	14.42	kdd	2.12	2.13	2.12	2.12
baudio	39.77	39.02	39.02	39.04	kosarek	10.60	10.71	10.56	10.55
bbc	248.33	240.19	242.83	242.79	msnbc	6.03	6.14	6.05	6.05
bnetflix	56.27	55.49	55.31	55.36	msweb	9.73	9.68	9.62	9.60
book	33.83	33.67	33.75	33.55	nltcs	5.99	5.99	5.99	5.99
c20ng	151.47	148.24	148.17	148.28	plants	12.54	12.45	12.26	12.27
cr52	83.35	81.52	81.17	81.31	pumbs	22.40	27.67	23.71	23.70
cwebkb	151.84	150.21	147.77	147.75	tmovie	50.81	48.69	49.23	49.29
dna	79.05	95.64	84.91	84.58	tretail	10.84	10.85	10.82	10.81

Table: Mean negative log-likelihoods attained by CMPCs on the test sets of 20 density estimation datasets. Taken from [2, Table 1].

CMPCs trained and benchmarked entirely generatively. No light shed on training and benchmarking them discriminatively. Discriminative PCs are of interest as they can classify incomplete samples (marg queries).

(1) How well can CMPCs classify samples of Binary MNIST?

Discriminative loss: replace NLL loss with cross-entropy, i.e. let  $\{(\mathbf{x}_j,y_j)\}_{j=1}^M$  denote training data and compute

$$\begin{aligned} \arg\min_{\phi} \mathcal{L}(\phi) &= \arg\min_{\phi} \mathsf{CE}(\phi) \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log \left( p_{\phi}(y_{j}|\mathbf{x}_{j}) \right) \right] \\ &= \arg\min_{\phi} \left[ -\sum_{i=1}^{M} \log \left( \frac{\frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}_{j}, y_{j}|z_{i})}{\frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}_{j}|z_{i})} \right) \right]. \end{aligned}$$

CMPCs trained and benchmarked entirely generatively. No light shed on training and benchmarking them discriminatively. Discriminative PCs are of interest as they can classify incomplete samples (marg queries).

(1) How well can CMPCs classify samples of Binary MNIST?

Discriminative loss: replace NLL loss with cross-entropy, i.e. let  $\{(\mathbf{x}_j,y_j)\}_{j=1}^M$  denote training data and compute

$$\begin{aligned} \arg\min_{\phi} \mathcal{L}(\phi) &= \arg\min_{\phi} \mathsf{CE}(\phi) \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log \left( p_{\phi}(y_{j}|\mathbf{x}_{j}) \right) \right] \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log \left( \frac{\frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}_{j}, y_{j}|z_{i})}{\frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}_{j}|z_{i})} \right) \right]. \end{aligned}$$

CMPCs trained and benchmarked entirely generatively. No light shed on training and benchmarking them discriminatively. Discriminative PCs are of interest as they can classify incomplete samples (marg queries).

#### (1) How well can CMPCs classify samples of Binary MNIST?

Discriminative loss: replace NLL loss with cross-entropy, i.e. let  $\{(\mathbf{x}_j,y_j)\}_{j=1}^M$  denote training data and compute

$$\begin{aligned} \arg\min_{\phi} \mathcal{L}(\phi) &= \arg\min_{\phi} \mathsf{CE}(\phi) \\ &= \arg\min_{\phi} \left[ -\sum_{j=1}^{M} \log \left( p_{\phi}(y_{j}|\mathbf{x}_{j}) \right) \right] \\ &= \arg\min_{\phi} \left[ -\sum_{i=1}^{M} \log \left( \frac{\frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}_{j}, y_{j}|z_{i})}{\frac{1}{N} \sum_{i=1}^{N} p_{\phi}(\mathbf{x}_{j}|z_{i})} \right) \right]. \end{aligned}$$

(2) Can generative power be maintained if learned discriminatively?

Hybrid loss [1]:

$$\mathcal{L}_{\lambda}(\phi) = \lambda \cdot \mathsf{CE}(\phi) + (1 - \lambda) \cdot \mathsf{NLL}(\phi)$$

where  $\lambda \in [0,1]$  determines the extent to which we train discriminatively (cross-entropy) and generatively (negative log-likelihood).

We call these hybrid CMPCs:

- $\lambda = 0 \rightarrow \text{hybrid CMPC trained fully-generative}$
- ullet  $\lambda=1$  ullet hybrid CMPC trained fully-discriminative
- ullet  $\lambda=0.5 
  ightarrow$  hybrid CMPC trained with a mix of gen. and discrim.

Question: Is there some  $\lambda \in [0,1]$  such that the model does well generatively and discriminatively?

(2) Can generative power be maintained if learned discriminatively?

Hybrid loss [1]:

$$\mathcal{L}_{\lambda}(\phi) = \lambda \cdot \mathsf{CE}(\phi) + (1 - \lambda) \cdot \mathsf{NLL}(\phi)$$

where  $\lambda \in [0,1]$  determines the extent to which we train discriminatively (cross-entropy) and generatively (negative log-likelihood).

We call these hybrid CMPCs:

- $\lambda = 0 \rightarrow \text{hybrid CMPC trained fully-generative}$
- ullet  $\lambda=1$  ullet hybrid CMPC trained fully-discriminative
- $\lambda = 0.5 o$  hybrid CMPC trained with a mix of gen. and discrim.

Question: Is there some  $\lambda \in [0,1]$  such that the model does well generatively and discriminatively?

(2) Can generative power be maintained if learned discriminatively?

Hybrid loss [1]:

$$\mathcal{L}_{\lambda}(\phi) = \lambda \cdot \mathsf{CE}(\phi) + (1 - \lambda) \cdot \mathsf{NLL}(\phi)$$

where  $\lambda \in [0,1]$  determines the extent to which we train discriminatively (cross-entropy) and generatively (negative log-likelihood).

We call these hybrid CMPCs:

- ullet  $\lambda=0$   $\to$  hybrid CMPC trained fully-generative
- ullet  $\lambda=1$  ullet hybrid CMPC trained fully-discriminative
- $\bullet~\lambda=0.5 \rightarrow \mbox{hybrid CMPC}$  trained with a mix of gen. and discrim.

Question: Is there some  $\lambda \in [0,1]$  such that the model does well generatively and discriminatively?

# Part 4: Hybrid CMPCs (results)



Figure: Samples of Binary MNIST.

#### Some details:

- 50,000 training samples, 10,000 validation and 10,000 testing
- ullet 28 by 28 each, pixel values in  $\{0,1\}$ , i.e.  $\Omega_{\mathbf{X}}=\{0,1\}^{784}$
- 10 classes, i.e.  $\Omega_Y = \{0, \dots, 9\}$

# Part 4: Hybrid CMPCs (results)



Figure: Samples of Binary MNIST.

#### Some details:

- 50,000 training samples, 10,000 validation and 10,000 testing
- 28 by 28 each, pixel values in  $\{0,1\}$ , i.e.  $\Omega_{\mathbf{X}} = \{0,1\}^{784}$
- 10 classes, i.e.  $\Omega_Y = \{0, \dots, 9\}$

Dewi Batista Hybrid CMPCs July 18, 2025

## Part 4: Hybrid CMPCs (classification results)

Six hybrid CMPCs trained, one for each  $\lambda \in \{0, 0.2, 0.4, 0.6, 0.8, 1\}$ , with:

- Latent dimension d=16, so  $\mathbf{Z} \sim \mathcal{N}(0,I_{16})$  and  $\phi: \mathbb{R}^{16} \to [0,1]^{784}$
- $N_{\text{train}} = 2^{13}$  components during training

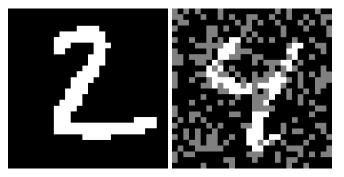


Figure: Samples of Binary MNIST. Left: A regular sample. Right: A sample pertaining to the digit 4 in which 30% of pixel values are missing at random.

# Part 4: Hybrid CMPCs (classification results)

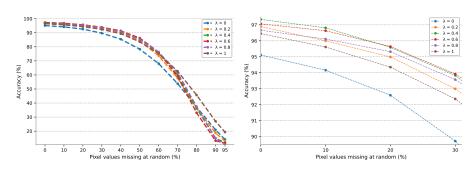


Figure: Classification accuracies of hybrid CMPCs trained on Binary MNIST for  $\lambda \in \{0, 0.2, 0.4, 0.6, 0.8, 1\}$  with differing portions of missing pixel values.

#### Surprising result

The hybrid CMPC trained with  $\lambda=0.4$  performs the best during classification, not the one trained entirely discriminatively (with  $\lambda=1$ ).

## Part 4: Hybrid CMPCs (classification results)

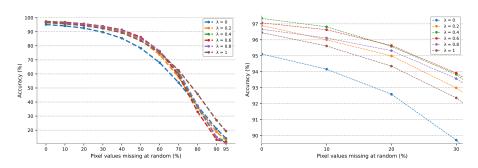


Figure: Classification accuracies of hybrid CMPCs trained on Binary MNIST for  $\lambda \in \{0, 0.2, 0.4, 0.6, 0.8, 1\}$  with differing portions of missing pixel values.

#### Surprising result

The hybrid CMPC trained with  $\lambda=0.4$  performs the best during classification, not the one trained entirely discriminatively (with  $\lambda=1$ ).

# Part 4: Hybrid CMPCs (sampling results)

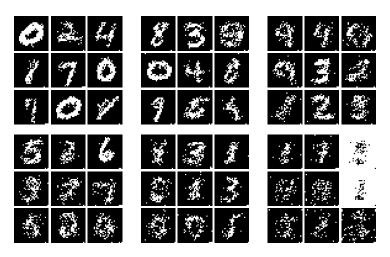


Figure: Samples of Binary MNIST drawn from hybrid CMPCs with d=16 and  $\lambda \in \{0,0.2,0.4,0.6,0.8,1\}$  ordered left-to-right top-to-bottom.

#### Discussion & Conclusion

#### Contributions:

- Beginner-friendly overviews of PCs and CMPCs, of which there are currently none
- 2 Experimentation regarding learning CMPCs in a hybrid manner

#### Discussion & Conclusion

#### Contributions:

- Beginner-friendly overviews of PCs and CMPCs, of which there are currently none
- Experimentation regarding learning CMPCs in a hybrid manner

#### Main results:

- Highest classification accuracies given by  $\lambda = 0.4$ ; higher than  $\lambda = 1$
- ② Sample degradation is gradual, heavy pixelation from  $\lambda = 0.6$  upward. Trading generative ability for discriminative via  $\lambda$  is possible

Hybrid CMPCs July 18, 2025 22 / 22

#### Discussion & Conclusion

#### Contributions:

- Beginner-friendly overviews of PCs and CMPCs, of which there are currently none
- Experimentation regarding learning CMPCs in a hybrid manner

#### Main results:

- ${\bf 0}$  Highest classification accuracies given by  $\lambda=0.4;$  higher than  $\lambda=1$
- ${\bf 2}$  Sample degradation is gradual, heavy pixelation from  $\lambda=0.6$  upward. Trading generative ability for discriminative via  $\lambda$  is possible

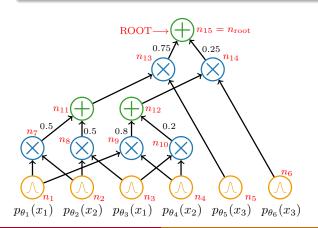
#### Future work:

- f 0 Fit more sophisticated PC structures fit to the N components
- Fit CMPCs to more sophisticated datasets, e.g. CIFAR-10

- [1] G. Bouchard and B. Triggs. The tradeoff between generative and discriminative classifiers. In *16th IASC International Symposium on Computational Statistics*, pages 721–728, 2004.
- [2] A. H. Correia, G. Gala, E. Quaeghebeur, C. de Campos, and R. Peharz. Continuous mixtures of tractable probabilistic models. In Proceedings of the AAAI Conference on Artificial Intelligence, volume 37, pages 7244–7252, 2023.
- [3] I. Goodfellow, Y. Bengio, and A. Courville. *Deep Learning*. MIT Press, 2016.
- [4] R. Peharz, R. Gens, F. Pernkopf, and P. Domingos. On the latent variable interpretation in sum-product networks. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 39(10):2030–2044, 2016.
- [5] D. Roth. On the hardness of approximate reasoning. *Artificial Intelligence*, 82(1-2):273–302, 1996.

#### Scope

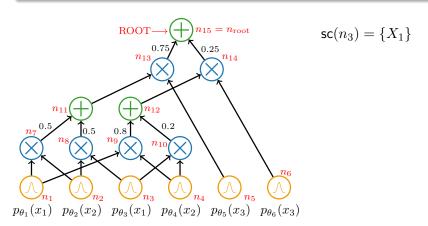
Recursively, the scope  $sc(n_i)$  of a sum or product node  $n_i$  is the union of the scopes of its parents. The scope of a input node is its corresponding subset of random variables in  $\mathbf{X}$ . By construction,  $sc(n_{root}) = \mathbf{X}$ .



 Dewi Batista
 Hybrid CMPCs
 July 18, 2025
 22 / 22

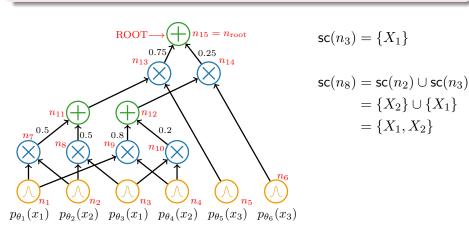
#### Scope

Recursively, the scope  $sc(n_i)$  of a sum or product node  $n_i$  is the union of the scopes of its parents. The scope of a input node is its corresponding subset of random variables in  $\mathbf{X}$ . By construction,  $sc(n_{root}) = \mathbf{X}$ .



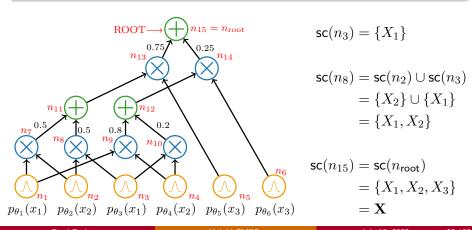
#### Scope

Recursively, the scope  $sc(n_i)$  of a sum or product node  $n_i$  is the union of the scopes of its parents. The scope of a input node is its corresponding subset of random variables in X. By construction,  $sc(n_{root}) = X$ .



#### Scope

Recursively, the scope  $sc(n_i)$  of a sum or product node  $n_i$  is the union of the scopes of its parents. The scope of a input node is its corresponding subset of random variables in  $\mathbf{X}$ . By construction,  $sc(n_{root}) = \mathbf{X}$ .



 Dewi Batista
 Hybrid CMPCs
 July 18, 2025
 22 / 22

### Appendix: Smoothness

#### **Smoothness**

A PC is smooth if for any sum node in  $\mathcal{G}$ , the scopes of its parents are equal.

#### Appendix: Smoothness

#### **Smoothness**

A PC is smooth if for any sum node in  $\mathcal{G}$ , the scopes of its parents are equal.

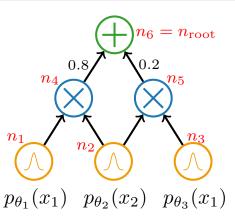


Figure: A smooth PC.

Example:  $\mathbf{pa}(n_6) = \{n_4, n_5\}$ ,  $\mathsf{sc}(n_4) = \{X_1, X_2\}$  and  $\mathsf{sc}(n_5) = \{X_1, X_2\}$ 

## Appendix: Decomposability

#### Decomposability

A PC is decomposable if for any product node in  $\mathcal{G}$ , the scopes of its parents are pairwise disjoint.

## Appendix: Decomposability

#### Decomposability

A PC is decomposable if for any product node in  $\mathcal{G}$ , the scopes of its parents are pairwise disjoint.

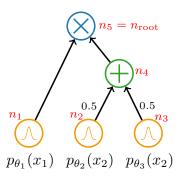


Figure: A decomposable PC.

Example:  $\mathbf{pa}(n_5) = \{n_1, n_4\}$ ,  $\mathrm{sc}(n_1) = \{X_1\}$  and  $\mathrm{sc}(n_4) = \{X_2\}$ 

## Appendix: Decomposability

#### Decomposability

A PC is decomposable if for any product node in  $\mathcal{G}$ , the scopes of its parents are pairwise disjoint.

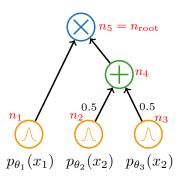


Figure: A decomposable PC.

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in sc(sum node)$ :

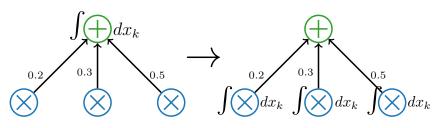


Figure: An integral being pushed down from a sum node to its parents.

$$\int_{\Omega_{X_2}} \sum_{i=1}^3 p_i(x_1, x_2, x_3) dx_2 \longrightarrow \sum_{i=1}^3 \int_{\Omega_{X_2}} p_i(x_1, x_2, x_3) dx_2$$

### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in sc(sum node)$ :

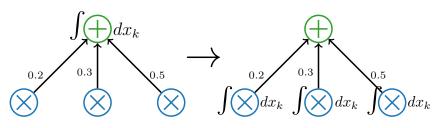


Figure: An integral being pushed down from a sum node to its parents.

$$\int_{\Omega_{X_2}} \sum_{i=1}^3 p_i(x_1, x_2, x_3) dx_2 \longrightarrow \sum_{i=1}^3 \int_{\Omega_{X_2}} p_i(x_1, x_2, x_3) dx_2$$

### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in sc(sum node)$ :

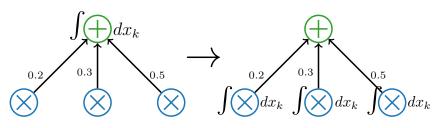


Figure: An integral being pushed down from a sum node to its parents.

$$\int_{\Omega_{X_2}} \sum_{i=1}^3 p_i(x_1, x_2, x_3) dx_2 \longrightarrow \sum_{i=1}^3 \int_{\Omega_{X_2}} p_i(x_1, x_2, x_3) dx_2$$

### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in \mathsf{sc}(\mathsf{product} \mathsf{ node})$ :

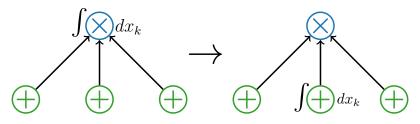


Figure: An integral being pushed down from a product node to one of its parents.

$$\int_{\Omega_{X_2}} p_1(x_1,x_2) p_2(x_3,x_4) p_3(x_5) dx_2 \rightarrow p_2(x_3,x_4) p_3(x_5) \int_{\Omega_{X_2}} p_1(x_1,x_2) dx_2$$

### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in \mathsf{sc}(\mathsf{product} \mathsf{ node})$ :

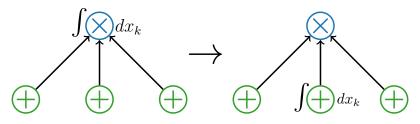


Figure: An integral being pushed down from a product node to one of its parents.

$$\int_{\Omega_{X_2}} p_1(x_1,x_2) p_2(x_3,x_4) p_3(x_5) dx_2 \rightarrow p_2(x_3,x_4) p_3(x_5) \int_{\Omega_{X_2}} p_1(x_1,x_2) dx_2$$

### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in \mathsf{sc}(\mathsf{product} \mathsf{ node})$ :

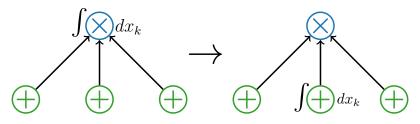


Figure: An integral being pushed down from a product node to one of its parents.

$$\int_{\Omega_{X_2}} p_1(x_1,x_2) p_2(x_3,x_4) p_3(x_5) dx_2 \rightarrow p_2(x_3,x_4) p_3(x_5) \int_{\Omega_{X_2}} p_1(x_1,x_2) dx_2$$

#### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in sc(input node)$ :

$$\int \int \int dx_k = 1$$

Figure: An integral being evaluated over the associated function of an input node.

$$\int_{\Omega_{X_2}} p_{\theta_z}(x_2) dx_2 \longrightarrow 1$$

#### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

For  $X_k \in sc(input node)$ :

$$\int \int \int dx_k = 1$$

Figure: An integral being evaluated over the associated function of an input node.

$$\int_{\Omega_{X_2}} p_{\theta_z}(x_2) dx_2 \longrightarrow 1$$

#### Purpose of smoothness and decomposability

The associated function  $p_{n_{\text{root}}}: \Omega_{\mathbf{X}} \to \mathbb{R}_{\geq 0}$  of the root node of a smooth and decomposable PC  $(\mathbf{X}, p_{(\mathcal{G}, \mathbf{w}, \theta)})$  is a probability function over  $\mathbf{X}$ .

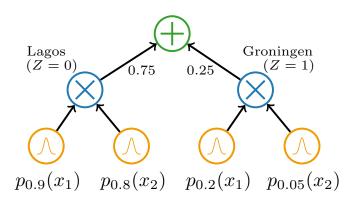
For  $X_k \in sc(input node)$ :

$$\int \int \int dx_k = 1$$

Figure: An integral being evaluated over the associated function of an input node.

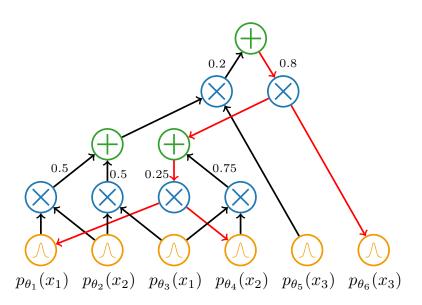
$$\int_{\Omega_{X_2}} p_{\theta_z}(x_2) dx_2 \longrightarrow 1$$

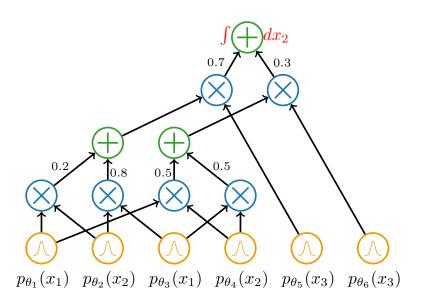
# Appendix: LVM interpretation of PCs [4]



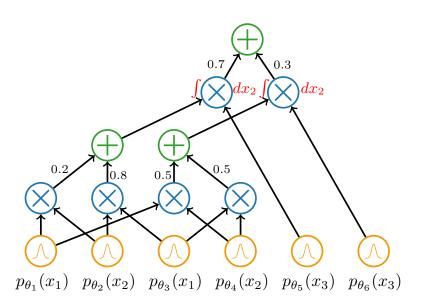
The latent variable  ${\bf Z}\sim {\sf Ber}(0.25)$  pertains to location of data recording and is marginalised out.

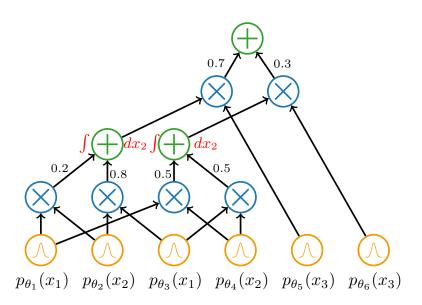
## Appendix: Sampling from a PC

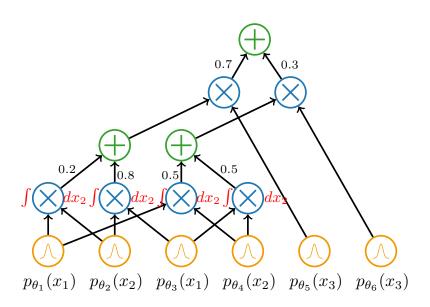


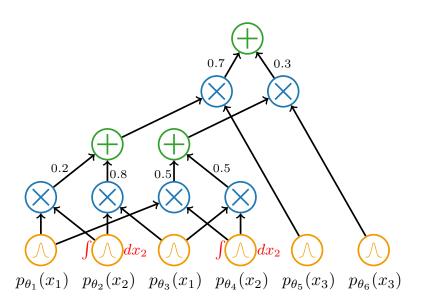


 Dewi Batista
 Hybrid CMPCs
 July 18, 2025
 22 / 22









 Dewi Batista
 Hybrid CMPCs
 July 18, 2025
 22 / 22

